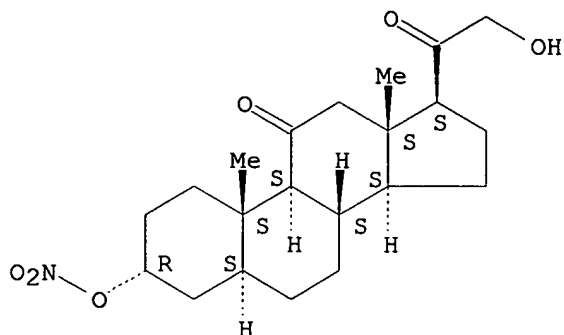


L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 21-hydroxy-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
 MF C21 H31 N O6

Absolute stereochemistry.

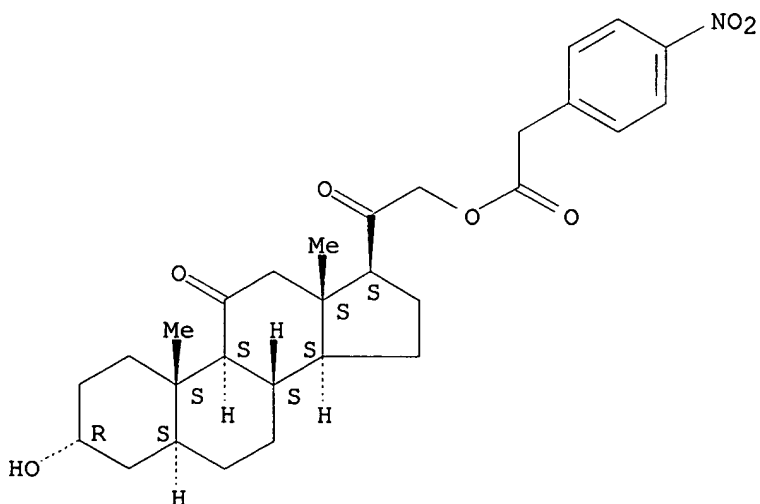


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):17

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 3-hydroxy-21-[[(4-nitrophenyl) acetyl]oxy]-, (3.alpha.,5.alpha.)- (9CI)
 MF C29 H37 N O7

Absolute stereochemistry.

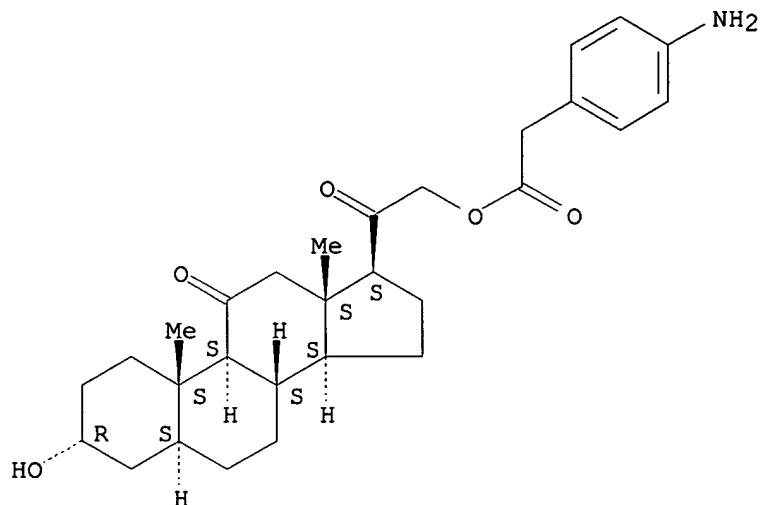


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 21-[[(4-aminophenyl) acetyl]oxy]-3-hydroxy-, (3.alpha.,5.alpha.)- (9CI)
 MF C29 H37 N O7

(3.alpha.,5.alpha.)- (9CI)
 MF C29 H39 N O5

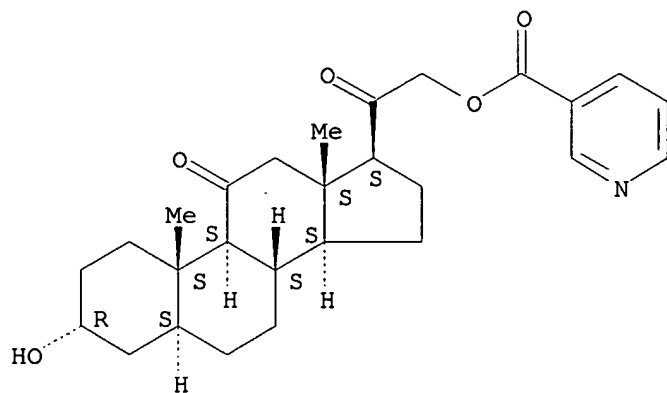
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 3-hydroxy-21-[(3-pyridinylcarbonyl)oxy]-,
 (3.alpha.,5.alpha.)- (9CI)
 MF C27 H35 N O5

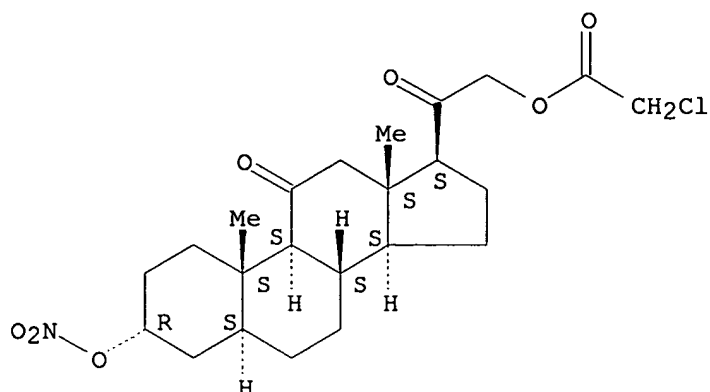
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 21-[(chloroacetyl)oxy]-3-(nitrooxy)-,
 (3.alpha.,5.alpha.)- (9CI)
 MF C23 H32 Cl N O7

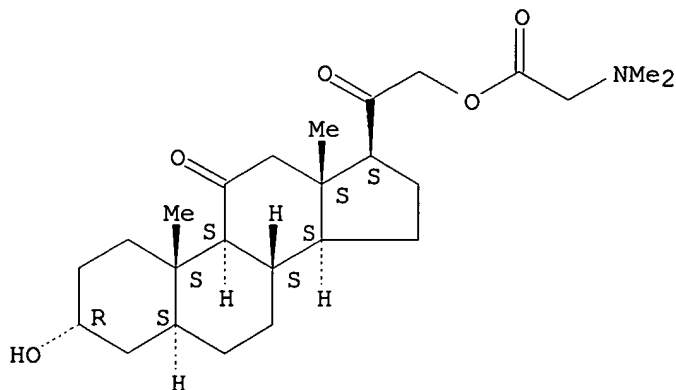
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, N,N-dimethyl-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-
 21-yl ester (9CI)
 MF C25 H39 N O5

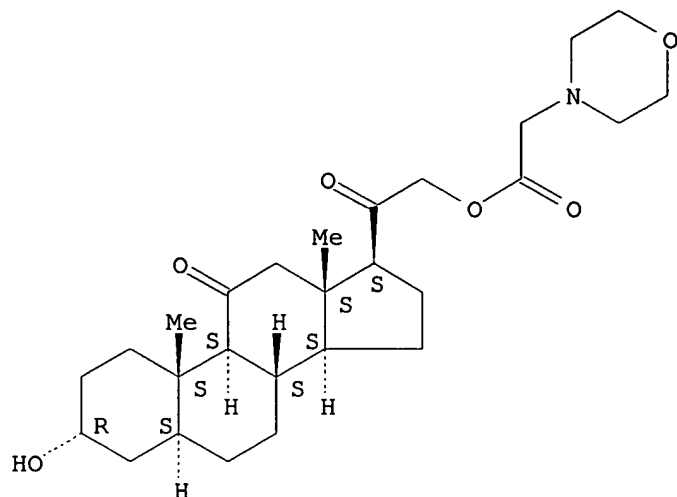
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 3-hydroxy-21-[(4-morpholinylacetyl)oxy]-,
 (3.alpha.,5.alpha.)- (9CI)
 MF C27 H41 N O6

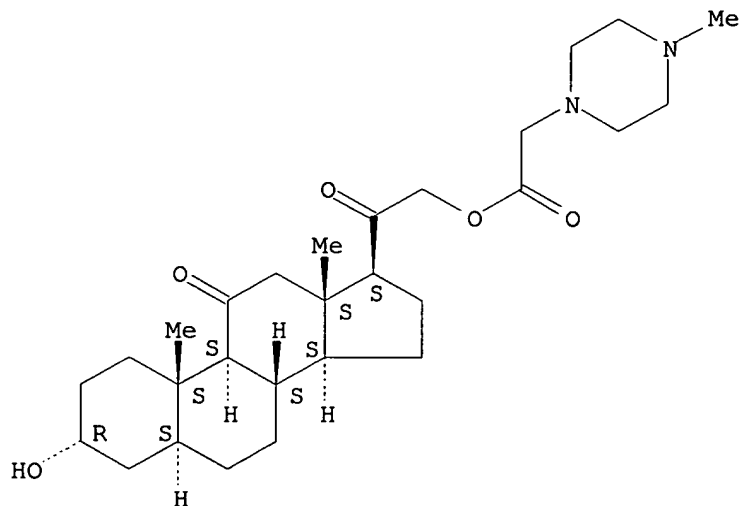
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 3-hydroxy-21-[[4-methyl-1-piperazinyl]acetyl]oxy-,
 (3.alpha.,5.alpha.)- (9CI)
 MF C28 H44 N2 O5

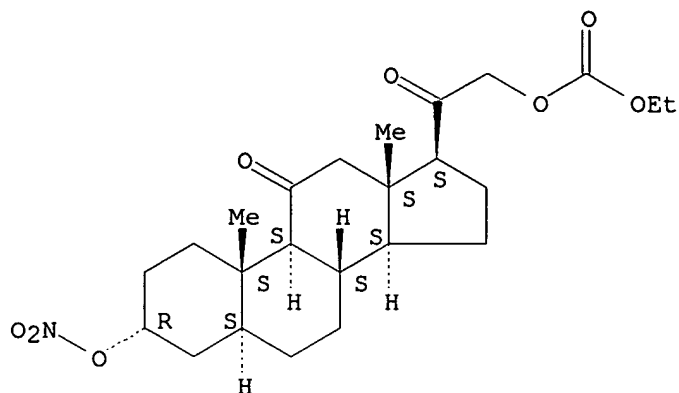
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 21-[(ethoxycarbonyl)oxy]-3-(nitrooxy)-,
 (3.alpha.,5.alpha.)- (9CI)
 MF C24 H35 N O8

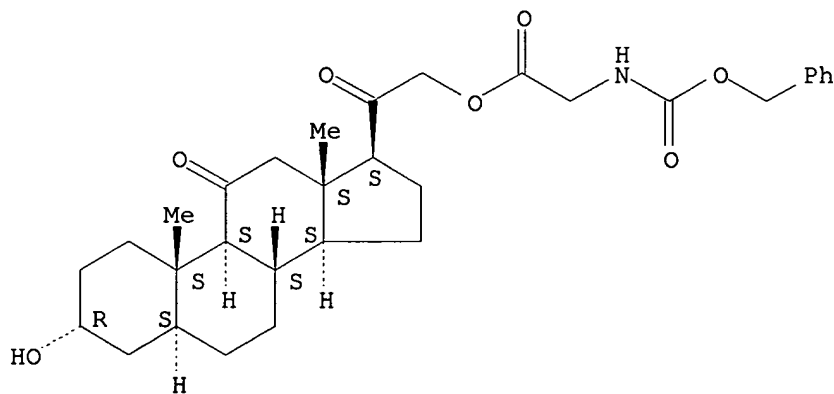
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, N-[(phenylmethoxy)carbonyl]-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-
 dioxopregnan-21-yl ester (9CI)
 MF C31 H41 N O7

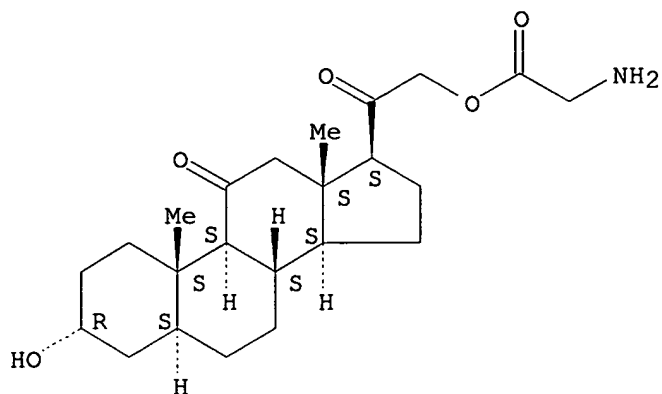
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester,
 hydrochloride (9CI)
 MF C23 H35 N O5 . Cl H

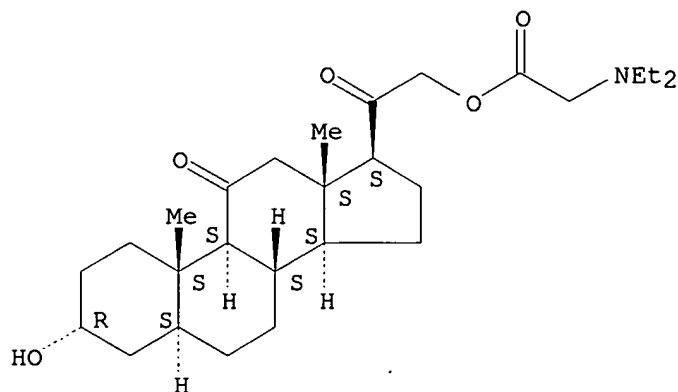
Absolute stereochemistry.



● HCl

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, N,N-diethyl-, (3.alpha.,5.alpha.)-3-hydroxy-11,20-dioxopregnan-21-yl ester (9CI)
 MF C27 H43 N O5

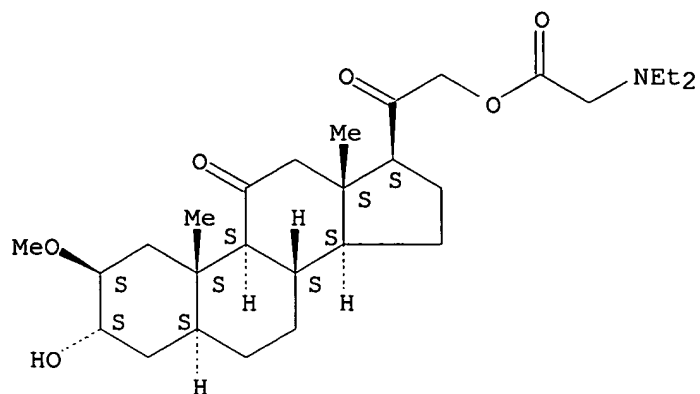
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, N,N-diethyl-, (2.beta.,3.alpha.,5.alpha.)-3-hydroxy-2-methoxy-11,20-dioxopregnan-21-yl ester (9CI)
 MF C28 H45 N O6

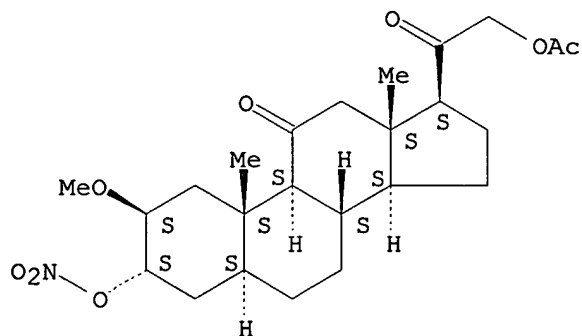
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 21-(acetyloxy)-2-methoxy-3-(nitrooxy)-,
 (2.β.,3.α.,5.α.)- (9CI)
 MF C24 H35 N O8

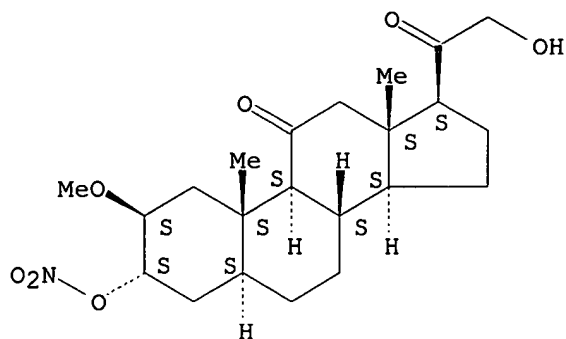
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenolone-11,20-dione, 21-hydroxy-2-methoxy-3-(nitrooxy)-,
 (2.β.,3.α.,5.α.)- (9CI)
 MF C22 H33 N O7

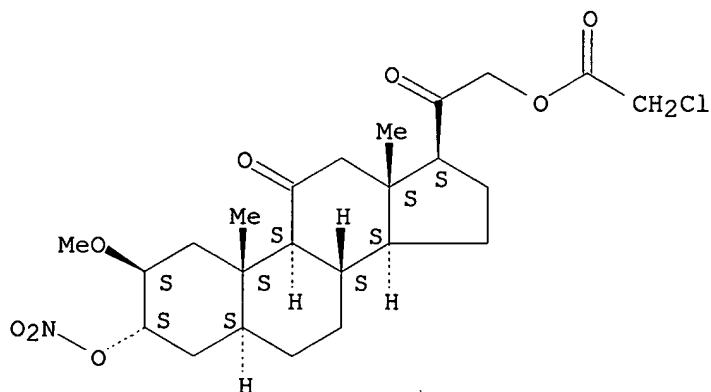
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 21-[(chloroacetyl)oxy]-2-methoxy-3-(nitrooxy)-,
 (2.beta.,3.alpha.,5.alpha.)- (9CI)
 MF C24 H34 Cl N O8

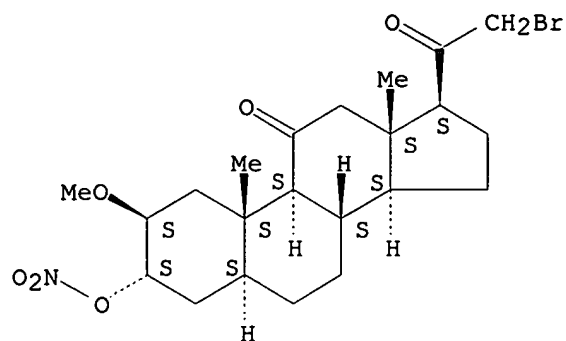
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 21-bromo-2-methoxy-3-(nitrooxy)-,
 (2.beta.,3.alpha.,5.alpha.)- (9CI)
 MF C22 H32 Br N O6

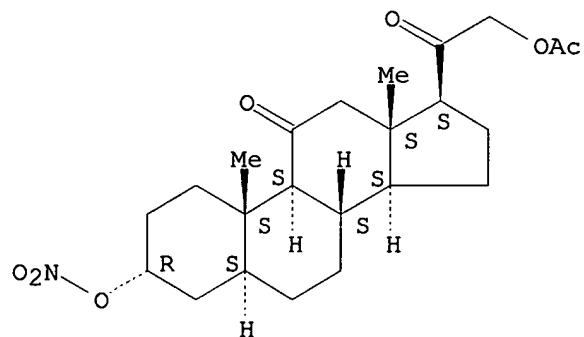
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 18 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnenone-11,20-dione, 21-(acetyloxy)-3-(nitrooxy)-, (3.alpha.,5.alpha.)-
 (9CI)
 MF C23 H33 N O7

Absolute stereochemistry.

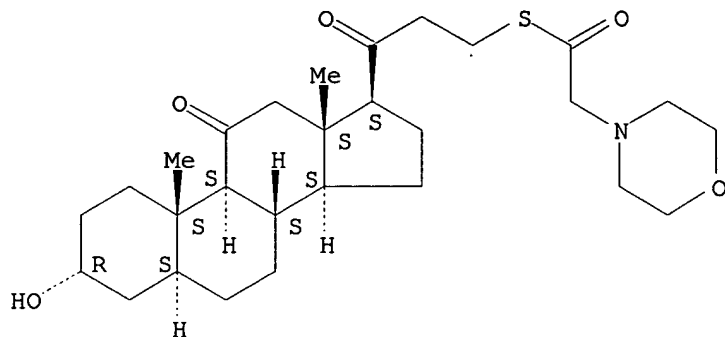


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-[(4-morpholinylacetyl)thio]-1-oxopropyl]-
 , (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C28 H43 N O5 S

Absolute stereochemistry.



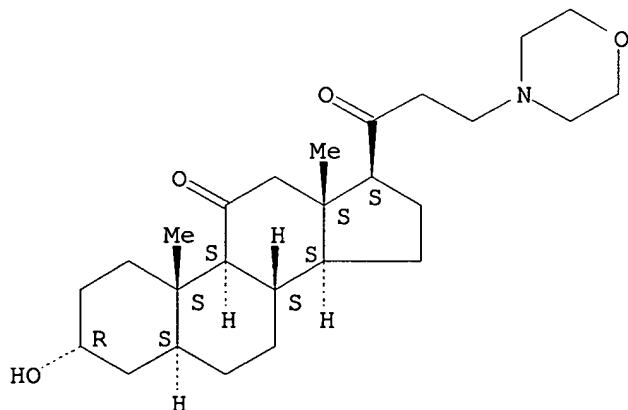
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):28

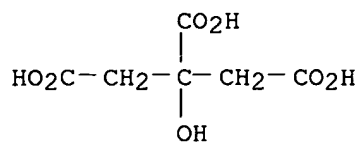
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-,
 (3.alpha.,5.alpha.,17.beta.)-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1)
 (9CI)
 MF C26 H41 N O4 . 1/3 C6 H8 O7

CM 1

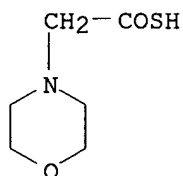
Absolute stereochemistry.



CM 2



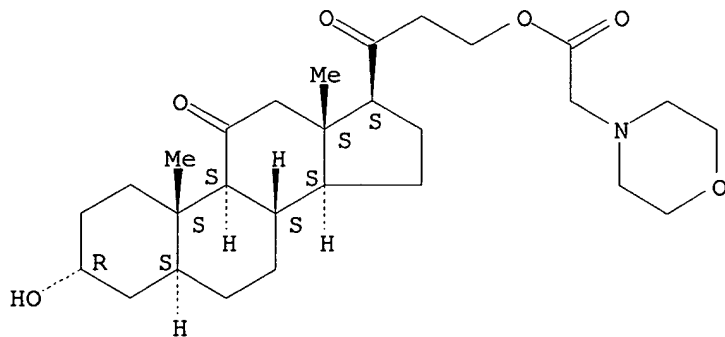
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 4-Morpholineethanethioic acid (9CI)
 MF **C6 H11 N O2 S**



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

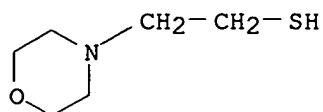
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-[(4-morpholinylacetyl)oxy]-1-oxopropyl]-
 , (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C28 H43 N O6**

Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

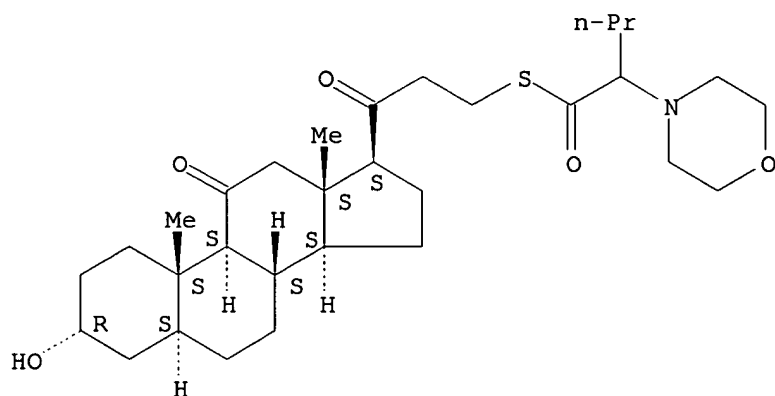
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 4-Morpholineethanethiol (6CI, 7CI, 8CI, 9CI)
 MF **C6 H13 N O S**
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

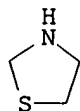
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-[[2-(4-morpholinyl)-1-oxopentyl]thio]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C31 H49 N O5 S**

Absolute stereochemistry.



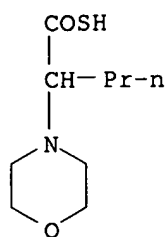
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Thiazolidine (6CI, 7CI, 8CI, 9CI)
 MF **C3 H7 N S**
 CI COM, RPS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

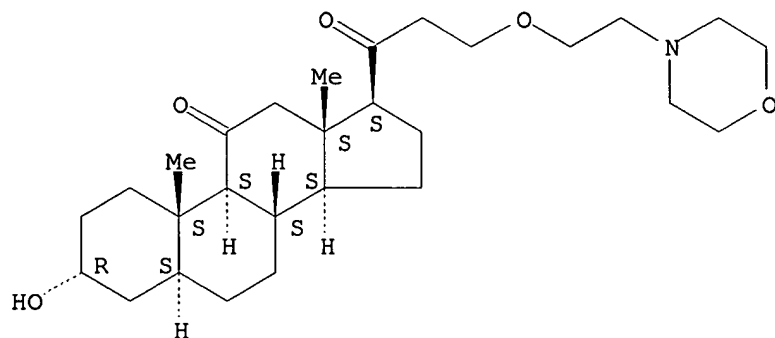
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 4-Morpholineethanethioic acid, .alpha.-propyl- (9CI)
 MF **C9 H17 N O2 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-[2-(4-morpholinyl)ethoxy]-1-oxopropyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C28 H45 N O5

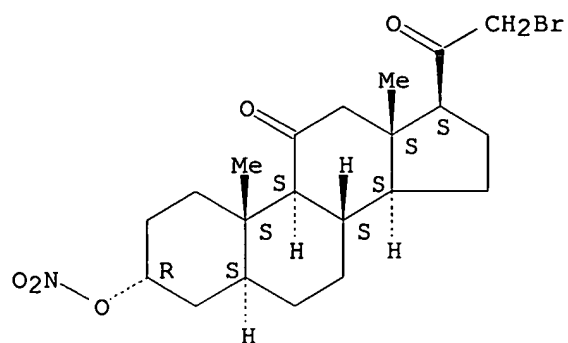
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnane-11,20-dione, 21-bromo-3-(nitrooxy)-, (3.alpha.,5.alpha.)- (9CI)
 MF C21 H30 Br N O5

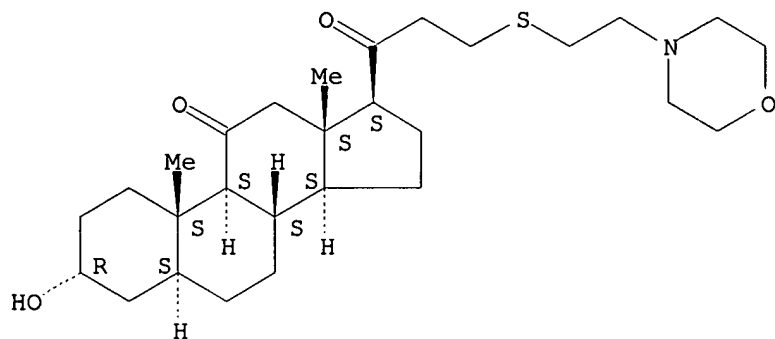
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

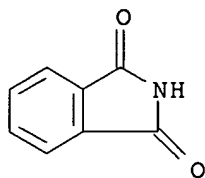
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-[[2-(4-morpholinyl)ethyl]thio]-1-oxopropyl]-, (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C28 H45 N O4 S**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

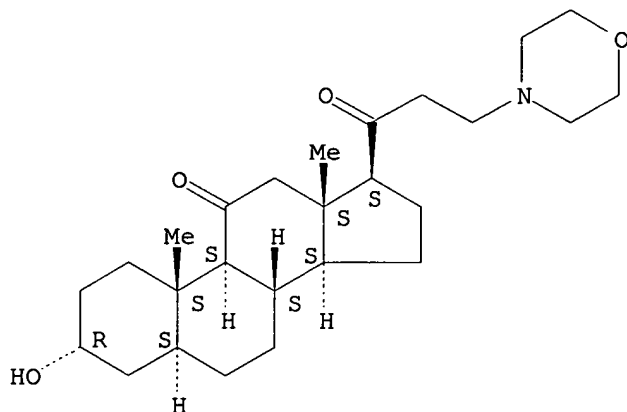
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 1H-Isoindole-1,3(2H)-dione, potassium salt (9CI)
 MF **C8 H5 N O2 . K**
 CI COM



● K

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C26 H41 N O4**
 CI COM

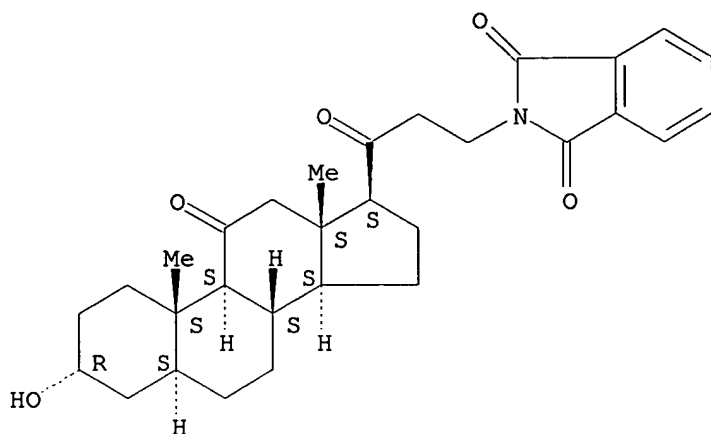
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

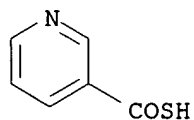
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 1H-Isoindole-1,3(2H)-dione, 2-[3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-
 11-oxoandrostan-17-yl]-3-oxopropyl]- (9CI)
 MF **C30 H37 N O5**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

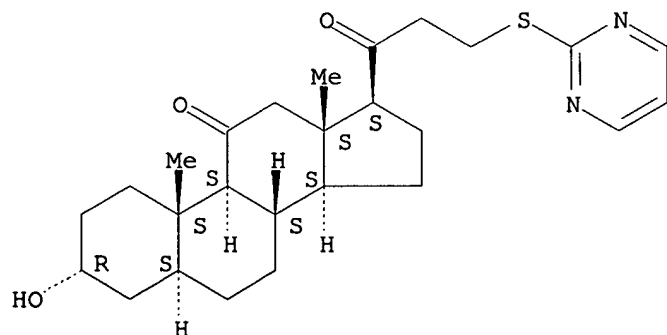
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 3-Pyridinecarbothioic acid (9CI)
 MF **C6 H5 N O S**
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

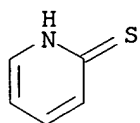
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(2-pyrimidinylthio)propyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C26 H36 N2 O3 S**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

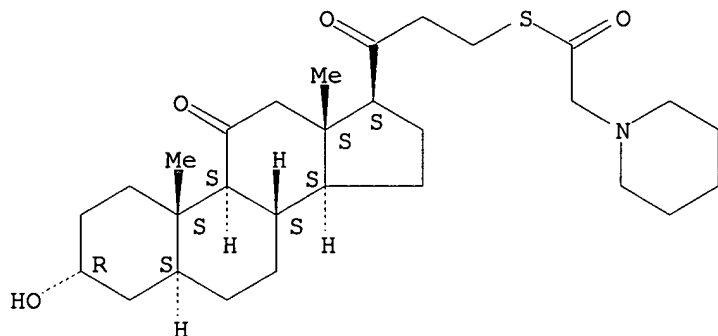
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 2(1H)-Pyridinethione (6CI, 7CI, 8CI, 9CI)
 MF **C5 H5 N S**
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-[(1-piperidinylacetyl)thio]propyl]-
 , (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C29 H45 N O4 S**

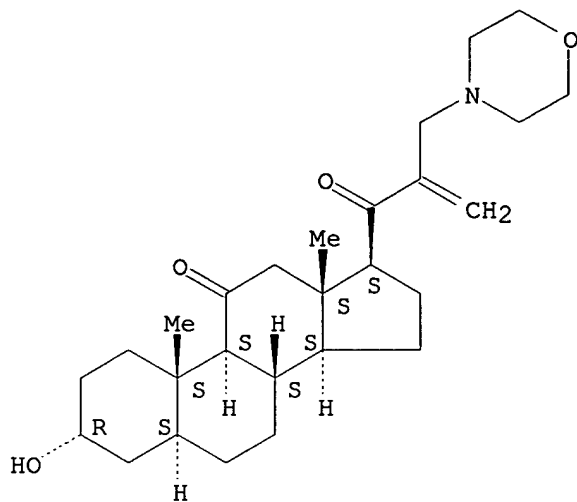
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

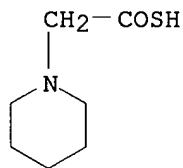
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[2-(4-morpholinylmethyl)-1-oxo-2-propenyl]-
 , (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF **C27 H41 N O4**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

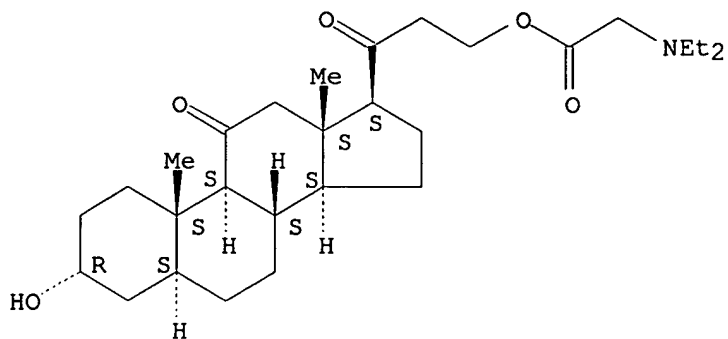
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 1-Piperidineethanethioic acid (9CI)
 MF C7 H13 N O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Glycine, N,N-diethyl-, 3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-oxopropyl ester (9CI)
 MF C28 H45 N O5

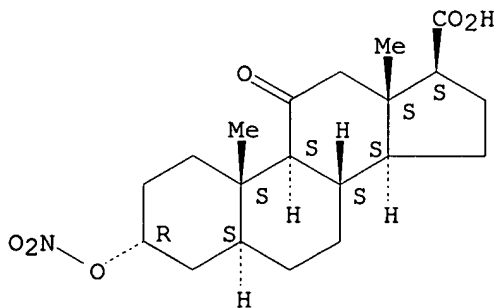
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstane-17-carboxylic acid, 3-(nitrooxy)-11-oxo-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C20 H29 N O6

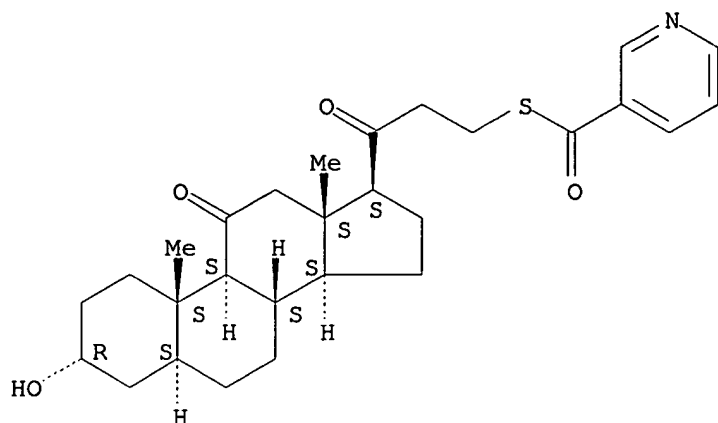
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

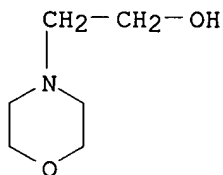
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-[(3-pyridinylcarbonyl)thio]propyl]-
 , (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C28 H37 N O4 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

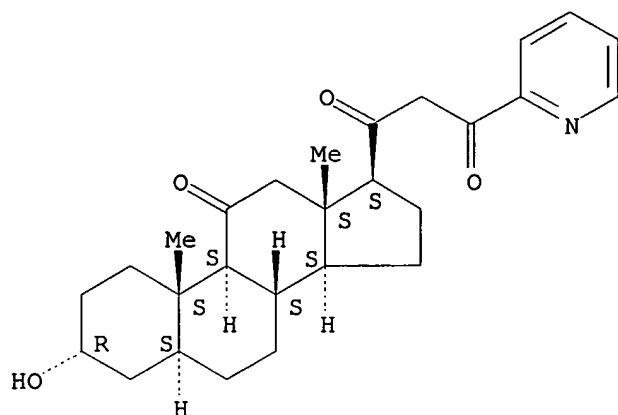
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 4-Morpholineethanol (6CI, 7CI, 8CI, 9CI)
 MF **C6 H13 N O2**
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 1,3-Propanedione, 1-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-11-oxoandrostan-17-yl]-3-(2-pyridinyl)- (9CI)
 MF **C27 H35 N O4**

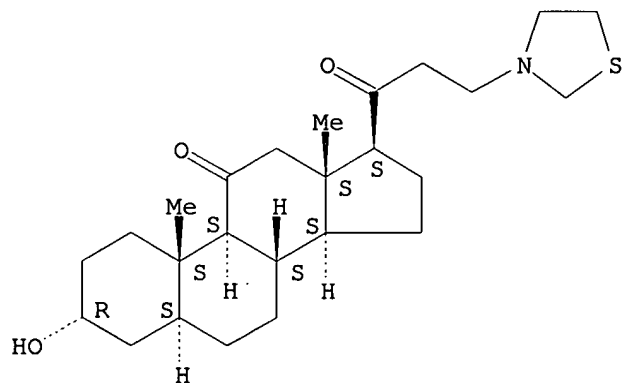
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(3-thiazolidinyl)propyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C25 H39 N O3 S

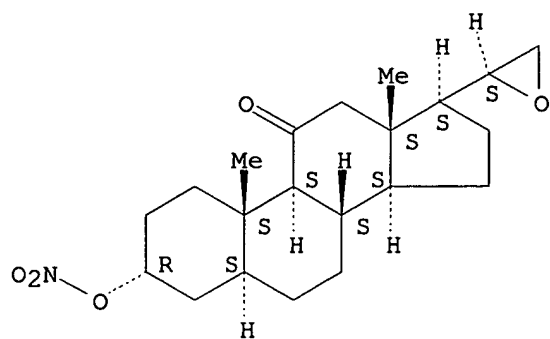
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Pregnan-11-one, 20,21-epoxy-3-(nitrooxy)-, (3.alpha.,5.alpha.,20S)- (9CI)
 MF C21 H31 N O5

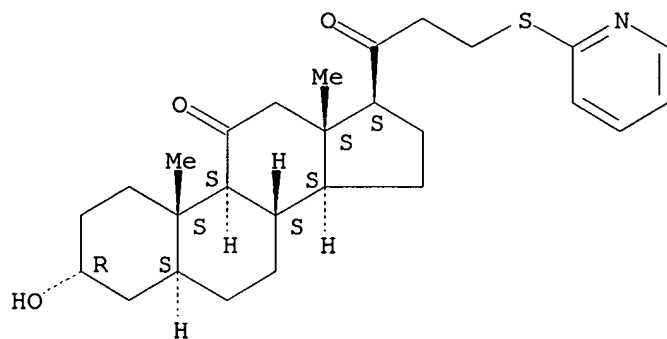
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

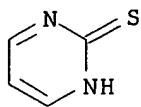
L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(2-pyridinylthio)propyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI)
 MF C27 H37 N O3 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 29 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
 IN 2(1H)-Pyrimidinethione (8CI, 9CI)
 MF C4 H4 N2 S
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d ibib ab hitstr 1-2

L10 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:450892 CAPLUS
DOCUMENT NUMBER: 131:102428
TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA
SOURCE: U.S., 28 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5925630	A	19990720	US 1996-659192	19960606
CA 2223996	AA	19961219	CA 1996-2223996	19960606
CN 1190404	A	19980812	CN 1996-195360	19960606
EP 1288220	A2	20030305	EP 2002-25321	19960606

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL

PRIORITY APPLN. INFO.: US 1995-467404 A2 19960606
EP 1996-919372 A3 19961219

OTHER SOURCE(S):

MARPAT 131:102428

AB Neuroactive steroids of formula I [R = H, NH₂, thio, sulfinyl, sulfonyl, halo, alkoxy, alkyl, alkenyl, alkynyl, etc.; R₁ = H, alkyl, alkenyl, alkynyl, haloalkyl, aryl, etc.; R₂ = H, alkoxy, keto, Me₂N; R₃ = alkoxy, alkenyloxy, alkynyloxy; R₄ = H, Me; R₅ = H, absent; R₆ = H, alkanoyl, etc.; R₇ = H, halo, OH, alkoxy, etc.; R₈ = H, halo; R₉ = H, halo, alkyl, alkoxy, arylalkoxy, amino; R₁₀ = H, halo, alkyl, OH, alkoxy, CN, etc.] are prepd. These derivs. are capable of acting at a recently identified site on the GABA receptor complex (GRC), thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.β-methoxy-5.β-androstan-3-one to give II. II protected 87.5% of mice injected with metrazol from convulsions.

IT 186264-69-7P

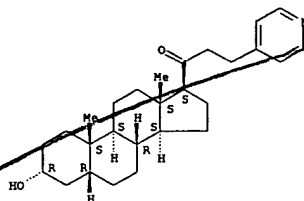
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of neuroactive steroids of androstane and pregnane series)

RN 186264-69-7 CAPLUS

CN 1-Propanone, 1-[(3.α.,5.β.,17.β.)-3-hydroxyandrostane-17-yl]-3-(4-pyridinyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:112239 CAPLUS
DOCUMENT NUMBER: 128:188632
TITLE: Use of GABA agonists and NMDA receptor antagonists for the treatment of migraine headache
INVENTOR(S): Lan, Nancy C.
PATENT ASSIGNEE(S): Cocensys, Inc., USA; Lan, Nancy C.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9805337	A1	19980212	WO 1997-US13430	19970731

V: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GR, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9739672 A1 19980225 AU 1997-39672 19970731
PRIORITY APPLN. INFO.: US 1996-22937P P 19960801
WO 1997-US13430 W 19970731

AB Methods are disclosed for treating or preventing migraine headache by administering to an animal a GABA receptor agonist (e.g. a neuroactive steroid) and/or an NMDA receptor antagonist (e.g. a dihydroquinoline deriv.). Also disclosed are pharmaceutical compns. and kits for the treatment or prevention of migraine headache.

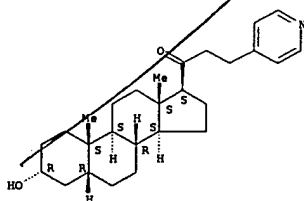
IT 186264-69-7

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(GABA agonists and NMDA receptor antagonists for migraine headache treatment)

RN 186264-69-7 CAPLUS

CN 1-Propanone, 1-[(3.α.,5.β.,17.β.)-3-hydroxyandrostane-17-yl]-3-(4-pyridinyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

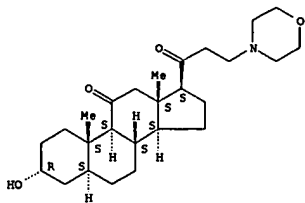


L10 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

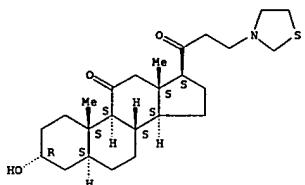
L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 CN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51228-28-5 CAPLUS
 CN Androstan-11-one, 3-hydroxy-17-[1-oxo-3-(3-thiazolidinyl)propyl]-,
 (3.alpha.,5.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

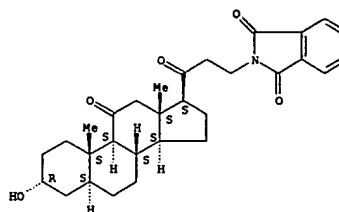
Absolute stereochemistry.



RN 51228-32-1 CAPLUS
 CN 1H-Indole-1,3(2H)-dione, 2-[3-[(3.alpha.,5.alpha.,17.beta.)-3-hydroxy-
 11-oxoandrostan-17-yl]-3-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

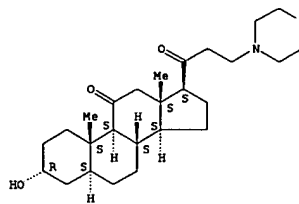


RN 51228-33-2 CAPLUS
 CN Androstan-11-one, 3-hydroxy-17-[3-(4-morpholinyl)-1-oxopropyl]-,
 (3.alpha.,5.alpha.,17.beta.)-, 2-hydroxy-1,2,3-propanetricarboxylate (3:1)
 (9CI) (CA INDEX NAME)

CM 1

CRN 51228-01-4
 CMF C26 H41 N O4

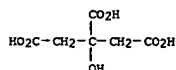
Absolute stereochemistry.



CM 2

CRN 77-92-9
 CMF C6 H8 O7

L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L10 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1972:514701 CAPLUS
 DOCUMENT NUMBER: 77:114701
 TITLE: 3.alpha.-Hydroxy-5.alpha.-pregnane-11,20-diones
 INVENTOR(S): Philipps, Gordon Hanley; Newall, Christopher Earle
 PATENT ASSIGNEE(S): Glaxo Laboratories Ltd.
 SOURCE: Ger. Offen., 45 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

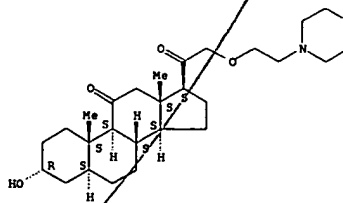
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2162594	A	19720706	DE 1971-2162594	19711216
NL 7117249	A	19720620	NL 1971-17249	19711216
FR 2118118	A5	19720728	FR 1971-45226	19711216
US 3882151	A	19751128	US 1971-208961	19711216
CA 995662	A1	19760824	CA 1971-130271	19711216
US 3969345	A	19760713	US 1975-551315	19750220
PRIORITY APPLN. INFO.:			GB 1970-60065	19701217
			US 1971-208961	19711216

AB Twenty title compds. [I, R = H2, O; R1 = H, Ac, O2N; R2 = H, Me; R3 = H, .beta.-MeO, .alpha.-OH, R4 = OMe, OEt, OCHMe2, O(CH2)2OMe, OC6H4NH2-p, O(CH2)2Cl, 2-morpholinoethoxy, 2-(4-methylpiperazinyl)ethoxy, O(CH2)2CN, O(CH2)2CO2Et, O(CH2)2Cl, O(CH2)2Cl, OCH2Ph, cyclohexyloxy], useful as anesthetics, were prepd. by methylation of the corresponding 21-diazo compd. Thus, 21-diazo-3.beta.-nitrate-5.alpha.-pregnane-11,20-dione in dry CH2Cl2-MeOH was refluxed with 14% Br2/MeOH 25 min to give I (R = O, R1 = NO2, R2 = R3 = H, R4 = OMe), which was stirred with Zn powder in HOAc 1.5 hr to give I (R = O, R1 = R2 = R3 = H, R4 = OMe).

IT 38601-40-0P 38601-41-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 38601-40-0 CAPLUS
 CN Pregnane-11,20-dione, 3-hydroxy-21-[2-(4-morpholinyl)ethoxy]-,
 (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 38601-41-1 CAPLUS
 CN Pregnane-11,20-dione, 3-hydroxy-21-[2-(4-methyl-1-piperazinyl)ethoxy]-,
 (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1970:404089 CAPLUS

DOCUMENT NUMBER: 73:4089

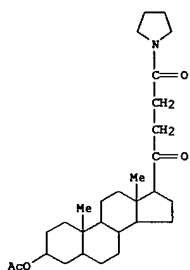
TITLE: Steroids and related natural products. 1. Bufadienolides. 4. Reaction of 20-oxo steroids with methoxymethyltriphenylphosphorane
 AUTHOR(S): Pettit, George R.; Green, Brian; Dunn, George L.; Sunder-Plassmann, Paul
 CORPORATE SOURCE: Dep. of Chem., Univ. of Maine, Orono, ME, USA
 SOURCE: Journal of Organic Chemistry (1970), 35(5), 1385-9
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Reaction of 3-hydroxy-20-oxo-5-pregnenes with the ylid prepd. from methoxy-methyltriphenylphosphonium chloride was studied in detail. 3.beta.-Acetoxy-20-methoxymethylene-5-pregnene (I) was also obtained along with a comparable amt. of 3.beta.-acetoxy-26,27-dinor-5,20(22)-cholestadiene, employing the mixt. of phosphoranes from methoxymethyltri-n-butylphosphonium chloride. Acid-catalyzed hydrolysis of vinyl ether I afforded the 20-aldehyde. Attempts to condense (methoxymethylene) triphenylphosphorane with Me 3.beta.-acetoxy-20-oxo-21-nor-5, trans-22-cholestadiene, its cis isomer, or Me 3.beta.-acetoxy-20-oxo-21-nor-5.alpha.-cholanate led to extensive side reactions attributable to the Me ester group. Use of the 3.beta.-tetrahydropyranyloxy-20-oxo-21-nor-5.alpha.-cholanate or tert-Bu 3.beta.-acetoxy-20-oxo-21-nor-5.alpha.-cholanate or the pyrrolidine amide eliminated side reactions but satisfactory involvement of the 20-ketone was not realized.

IT 23439-96-5P 23439-97-6P 23439-98-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 23439-96-5 CAPLUS

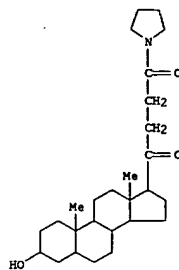
CN Pyrrolidine, 1-(3.beta.-hydroxy-20-oxo-21-nor-5.alpha.-cholan-24-oyl)-, acetate (ester) (8CI) (CA INDEX NAME)



RN 23439-97-6 CAPLUS

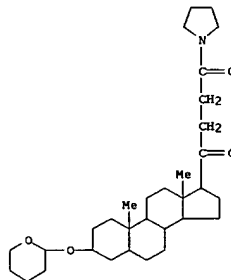
L10 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CN Pyrrolidine, 1-(3.beta.-hydroxy-20-oxo-21-nor-5.alpha.-cholan-24-oyl)- (8CI) (CA INDEX NAME)



RN 23439-98-7 CAPLUS

CN Pyrrolidine, 1-[20-oxo-3.beta.-[(tetrahydro-2H-pyran-2-yl)oxy]-21-nor-5.alpha.-cholan-24-oyl]- (8CI) (CA INDEX NAME)



L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1962:2568 CAPLUS

DOCUMENT NUMBER: 56:2568

ORIGINAL REFERENCE NO.: 56:530c-f

TITLE: Mannich bases of steroids and their salts

INVENTOR(S): Thiesing, Jan; Bork, Karl Heinz

PATENT ASSIGNEE(S): E. Merck A.-G.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1107662			DE	19590704

AB 178-Acetylsteroids were treated simultaneously or in turn with CH₂O and a secondary amine under the conditions of the Mannich reaction and the Mannich bases optionally treated with an acid to give the title compds. Thus, a mixt. of 7.17 5-pregnen-3.beta.-ol-20-one acetate, 1.2 paraformaldehyde, and 2.66 g. piperidinium chloride in 100 cc. tert-amyl alc. was refluxed 4 hrs. and the soln. cooled and dild. with Et₂O to give 21-piperidinomethyl-5-pregnen-3.beta.-ol-20-one. 3-acetate-HCl (I), m. 208-10.degree. (Me₂CO), [.alpha.]_D 20.0.degree.; free base (II), m. 140-2.degree. (MeOH), [.alpha.]_D 10.1.degree.; I on sapon. with concd. HCl gave 21-piperidinomethyl-5-pregnen-3.beta.-ol-20-one-HCl, m. 219-22.degree. (EtOH); free base (II), m. 168-70.degree., [.alpha.]_D 13.1.degree.. Similarly were prepd. the following Mannich bases or their salts (product, m. p., and [.alpha.]_D given): II maleate, 154-6.degree. (Me₂CO), 4.degree.; II camphorsulfonate, 193-4.degree., 15.5.degree.; II tartrate, 141.degree.; III succinate, 111-20.degree., 16.0.degree.; III succinate, 110-1.degree.; 21-piperidinomethyl-5,16-pregnadien-3.beta.-ol-20-one, 24.1.degree.; (EtOH), -42.6.degree.; 21-dimethylaminomethyl-5-pregnen-3.beta.-ol-20-one 3-acetate-HCl, 25.7.degree.; 21-pyrrolidinomethyl-5-pregnen-3.beta.-ol-20-one 3-acetate-HCl, 198-9.degree. [free base, 138-40.degree. (aq. EtOH); succinate 102-4.degree. (Me₂CO), 9.3.degree.]; 21-morpholinomethylallopregnan-3.beta.-ol-20-one 3-acetate-HCl, 197-9.degree. (iso-PrOH), 48.0.degree. [free base, 92-5.degree. (hexane), 56.0.degree.]; 16-methyl-21-piperidinomethyl-15-16-pregnadien-3.beta.-ol-20-one 3-acetate HCl, 213-16.degree. - [free base, 95-7.degree. (MeOH), -0.6.degree.].

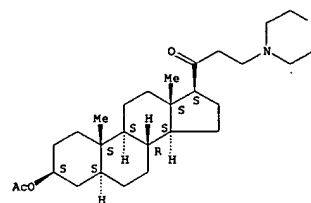
IT 103572-42-5, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-morpholino-, acetate, hydrochloride 103572-43-6, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-morpholino-, acetate 106481-73-6, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-piperidino-, acetate, hydrochloride 106481-74-7, 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-piperidino-, acetate (prepn. of)

RN 103572-42-5 CAPLUS

CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-morpholino-, acetate, hydrochloride (7CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

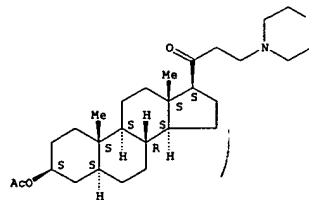


● HCl

RN 103572-43-6 CAPLUS

CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-morpholino-, acetate (7CI) (CA INDEX NAME)

Absolute stereochemistry.

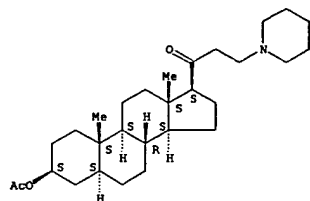


RN 106481-73-6 CAPLUS

CN 1-Propanone, 1-(3.beta.-hydroxy-5.alpha.-androst-17.beta.-yl)-3-piperidino-, acetate, hydrochloride (7CI) (CA INDEX NAME)

Absolute stereochemistry.

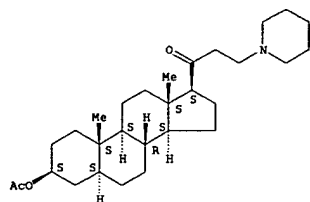
L10 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

RN 106481-74-7 CAPLUS
CN 1-Propanone, 1-(3.β.-hydroxy-5.α.-androst-17.β.-yl)-3-piperidino-, acetate (7CI) (CA INDEX NAME)

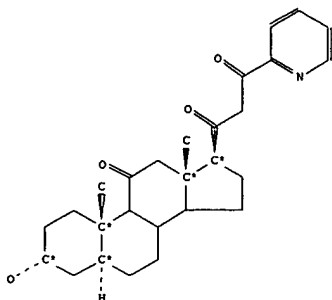
Absolute stereochemistry.



=> d all 1-13

L12 ANSWER 1 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1609851
 Beilstein Pref. RN (BPR): 51227-92-0
 CAS Reg. No. (RN): 51227-92-0
 Chemical Name (CN): 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione
 Autonom Name (AUN): 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione
 Molec. Formula (MF): C27 H35 N O4
 Molecular Weight (MW): 437.58
 Lawson Number (LN): 26223
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1549260
 Tautomer ID (TAUTID): 1623273
 Beilstein Citation (BSO): 5-21
 Entry Date (DED): 1988/11/30
 Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1

L12 ANSWER 1 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

UV/VIS 11

Reference(s):

1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:

RX
 Reaction ID (.ID): 6850433
 Product BRN (.PBRN): 1609851
 Product (.PRO): 1-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-pyridin-2-yl-propane-1,3-dione
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 6850433.1
 Reaction Classification (.CL): Preparation (half reaction)
 Reference(s):
 1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 1 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

Code	Name	Occurrence
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FV	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

179 - 180 11

Reference(s):

1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYPE)	(.W)	1
(deg)		(nm)	

21.4 1(alpha) 589 11

Reference(s):

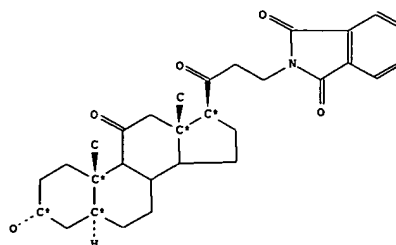
1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

UV and Visible Spectrum:

Description	Ref.
(.RV)	1

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1519724
 Beilstein Pref. RN (BPR): 51228-32-1
 CAS Reg. No. (RN): 51228-32-1
 Chemical Name (CN): 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione
 Autonom Name (AUN): 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione
 Molec. Formula (MF): C30 H37 N O5
 Molecular Weight (MW): 491.63
 Lawson Number (LN): 25776, 15890
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1481883
 Tautomer ID (TAUTID): 1539358
 Beilstein Citation (BSO): 5-21
 Entry Date (DED): 1988/11/30
 Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FV	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

187 - 189 |1

Reference(s):

1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYP)	(.W)	1
(deg)	1	(nm)	1

58.8 | [alpha] | 589 | 1

Reference(s):

1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:

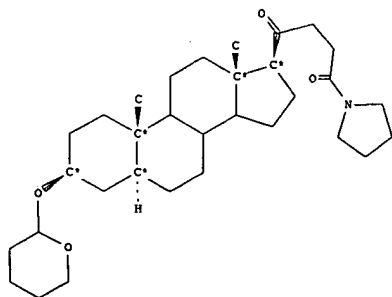
RX
 Reaction ID (.ID): 6647974
 Product BRN (.PBRN): 1519724
 Product (.PRO): 2-<3-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopentaca>phenanthren-17-yl)-3-oxo-propyl>-isoindole-1,3-dione
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 6647974.1
 Reaction Classification (.CL): Preparation (half reaction)
 Reference(s):
 1. Patent: Glaxo Lab. Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 3 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1412117
 Beilstein Pref. RN (BPR): 23439-98-7
 CAS Reg. No. (RN): 23439-98-7
 Chemical Name (CN): 1-<10,13-dimethyl-3-(tetrahydro-pyran-2-yloxy)-hexadecahydro-cyclopenta>phenanthren-17-yl>-4-pyrrolidin-1-yl-butane-1,4-dione
 Autonom Name (AUN): 1-<10,13-dimethyl-3-(tetrahydro-pyran-2-yloxy)-hexadecahydro-cyclopenta>phenanthren-17-yl>-4-pyrrolidin-1-yl-butane-1,4-dione
 Molec. Formula (MF): C32 H51 N O4
 Molecular Weight (MW): 513.76
 Lawson Number (LN): 24077, 17122, 13467
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1392251
 Tautomer ID (TAUTID): 1440908
 Beilstein Citation (BSO): 5-20
 Entry Date (DED): 1988/11/29
 Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1

L12 ANSWER 2 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

MF	Molecular Formula	1
FV	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

117 - 119 |1

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYP)	(.W)	1
(deg)	1	(nm)	1

65 | [alpha] | 589 | 1

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

Descript	Ref.
ion	1
(.KV)	1

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 3 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Reaction:

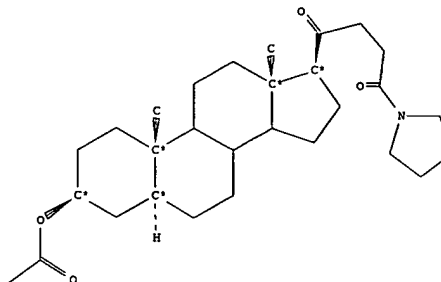
RX
Reaction ID (.ID): 6559028
Product BRN (.PBRN): 1412117
Product (.PRO): 1-(10,13-dimethyl-3-(tetrahydro-pyran-2-
yloxy)-hexadecahydro-
cyclopenta<a>phenanthren-17-yl)-4-
pyrrolidin-1-yl-butane-1,4-dione
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 6559028.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1410392
Beilstein Pref. RN (BPR): 23439-96-5
CAS Reg. No. (RN): 23439-96-5
Chemical Name (CN): acetic acid 10,13-dimethyl-17-(4-oxo-4-
pyrrolidin-1-yl-butyl)-hexadecahydro-
cyclopenta<a>phenanthren-3-yl ester
Autonom Name (AUN):
Molec. Formula (MF): C29 H45 N O4
Molecular Weight (MW): 471.68
Lawson Number (LN): 24077, 13467, 1155
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 1390379
Tautomer ID (TAUTID): 1442152
Beilstein Citation (BSO): 5-20
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Code	Name	Occurrence
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

124 - 125 11

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

Descript	Ref.
ion	1
(.KW)	1

IR 11

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Reaction:

RX
Reaction ID (.ID): 6557733
Product BRN (.PBRN): 1410392
Product (.PRO): acetic acid 10,13-dimethyl-17-(4-oxo-4-
pyrrolidin-1-yl-butyl)-hexadecahydro-
cyclopenta<a>phenanthren-3-yl ester
No. of React. Details (.NVAR): 1

Reaction Details:

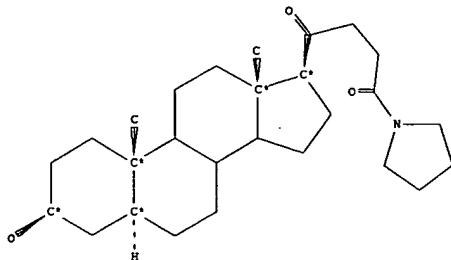
RX
Reaction RID (.RID): 6557733.1

L12 ANSWER 4 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1406458
 Beilstein Pref. RN (BPR): 23439-97-6
 CAS Reg. No. (RN): 23439-97-6
 Chemical Name (CN): 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione
 Autonom Name (AUN): 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione
 Molec. Formula (MF): C27 H43 N O3
 Molecular Weight (MW): 429.64
 Lawson Number (LN): 24077, 13467
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1388949
 Tautomer ID (TAUTID): 1438336
 Beilstein Citation (BSO): 5-20
 Entry Date (DED): 1988/11/29
 Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Reaction:
 RK
 Reaction ID (.ID): 6554710
 Product BRN (.PBRN): 1406458
 Product (.PRO): 1-(3-hydroxy-10,13-dimethyl-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-4-pyrrolidin-1-yl-butane-1,4-dione
 No. of React. Details (.NVAR): 1
 Reaction Details:
 RK
 Reaction RID (.RID): 6554710.1
 Reaction Classification (.CL): Preparation (half reaction)
 Reference(s):
 1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 5 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Code	Name	Occurrence
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	(Ref.)
(MP)	1
(Cel)	1

222 - 224 11

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Optical Rotatory Power:

Value	Type	Wavelength	(Ref.)
(ORP)	1 (.TYP)	1 (.W)	1
(deg)	1	1 (nm)	1

67 1(alpha) 1 589 11

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

Infrared Spectrum:

Descript	(Ref.)
ion	1
(.KW)	1

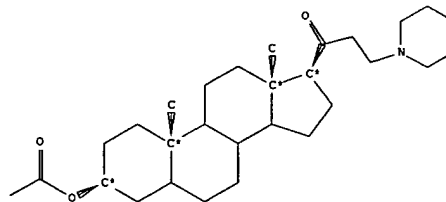
IR 11

Reference(s):

1. Pettit et al., J.Org.Chem., CODEN: JOCEAH, 35, <1970>, 1398

L12 ANSWER 6 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1356921
 Beilstein Pref. RN (BPR): 105481-74-7
 CAS Reg. No. (RN): 105481-74-7
 Chemical Name (CN): 3.beta.-Acetoxy-21-piperidinomethyl-allopregnan-20-on
 Autonom Name (AUN): acetic acid 10,13-dimethyl-17-(3-piperidin-1-yl-propionyl)-hexadecahydro-cyclopenta<a>phenanthren-3-yl ester
 Molec. Formula (MF): C29 H47 N O3
 Molecular Weight (MW): 457.70
 Lawson Number (LN): 24081, 15809, 1155
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1303936
 Tautomer ID (TAUTID): 1343478
 Beilstein Citation (BSO): 5-20
 Entry Date (DED): 1988/11/29
 Update Date (DUPD): 1991/03/25



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CDER	Chemical Derivative	2
FINFO	Further Information	1

L12 ANSWER 6 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

MF Melting Point 1
This substance also occurs in Reaction Documents:
Code Name Occurrence

RX Reaction Documents 1
RXPRO Substance is Reaction Product 1

Chemical Derivative:
CDER

Note(s) (.COM): Hydrochlorid: F: 180-182grad (Vasser)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

CDER Note(s) (.COM): Hydrogentartrat: F: 109-111grad (EtOH);
<.alpha.>(D) +44.0grad (Dioxan)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Melting Point:

Value [Ref.
(MP) |
(Cel)
96 - 97 |1

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Further Information:

FINFO Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Reaction:

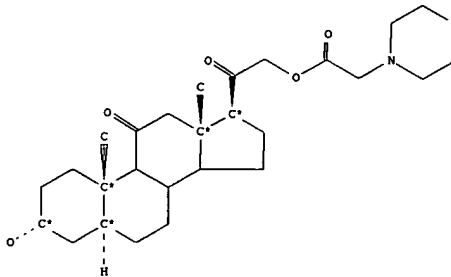
RX Reaction ID (.ID): 6514830
Product BRN (.PBRN): 1356921
Product (.PRO): 3.beta.-Acetoxy-21-piperidinomethyl-
allopregnan-20-on
No. of React. Details (.NVAR): 1

Reaction Details:

RX Reaction RID (.RID): 6514830.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1189841
Beilstein Pref. RN (BPR): 38392-79-9
CAS Reg. No. (RN): 38392-79-9
Chemical Name (CN): 3-hydroxy-21-(morpholin-4-yl-acetoxy)-
pregnane-11,20-dione
Autonom Name (AUN): morpholin-4-yl-acetic acid
2-(3-hydroxy-10,13-dimethyl-11-oxo-
hexadecahydro-cyclopenta<a>phenanthren-17-
yl)-2-oxo-ethyl ester
Molec. Formula (MF): C27 H41 N O6
Molecular Weight (MW): 475.62
Lawson Number (LN): 30824, 9769, 3379
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 1133480
Tautomer ID (TAUTID): 1155411
Beilstein Citation (BSO): 5-27
Entry Date (DED): 1988/11/29
Update Date (DUPD): 1992/04/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

FW Formular Weight 1
LN Lawson Number 3
FS File Segment 1
CTYPE Compound Type 1
CONSID Constitution ID 1
TAUTID Tautomer ID 1
BSO Beilstein Citation 1
ED Entry Date 1
UPD Update Date 1
MP Melting Point 1
ORP Optical Rotatory Power 1

This substance also occurs in Reaction Documents:

Code Name Occurrence

RX Reaction Documents 1
RXPRO Substance is Reaction Product 1

Melting Point:

Value [Ref.
(MP) |
(Cel)
131 - 133 |1

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

Value [Type [Wavelen. [Ref.
(ORP) | (.TYP) | (.W) |
(deg) | | (nm) |

87.5 | [alpha] | 589 | 1

Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

Reaction:

RX Reaction ID (.ID): 6382297
Product BRN (.PBRN): 1189841
Product (.PRO): 3-hydroxy-21-(morpholin-4-yl-acetoxy)-
pregnane-11,20-dione
No. of React. Details (.NVAR): 1

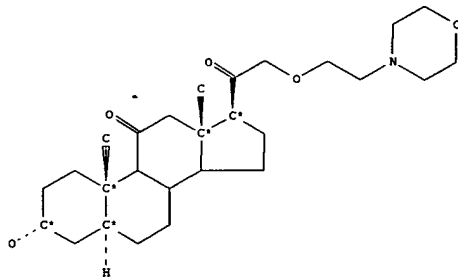
Reaction Details:

RX Reaction RID (.RID): 6382297.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(102035)

L12 ANSWER 7 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1182924
 Beilstein Pref. RN (BPR): 38601-40-0
 CAS Reg. No. (RN): 38601-40-0
 Chemical Name (CN): 3-hydroxy-21-(2-morpholin-4-yl-ethoxy)-pregnane-11,20-dione
 Autonom Name (AUN): 3-hydroxy-10,13-dimethyl-17-((2-morpholin-4-yl-ethoxy)-acetyl)-hexadecahydro-cyclopenta[*a*]phenanthren-11-one
 C27 H43 N O5
 Molec. Formula (MF):
 Molecular Weight (MW): 461.64
 Lawson Number (LN): 30824, 9769, 3122
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1131927
 Tautomer ID (TAUTID): 1151603
 Beilstein Citation (BSO): 5-27
 Entry Date (DED): 1988/11/29
 Update Date (DUPD): 1992/04/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1

L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

RX
 Reaction RID (.RID): 6377982.1
 Reaction Classification (.CL): Preparation (half reaction)
 Reference(s):
 1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

L12 ANSWER 8 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

112 - 113 11

Reference(s):

1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYP)	(.W)	1
(deg)		(nm)	1

72 1[alpha] 589 11

Reference(s):

1. Patent: Glaxo Lab. DE 2162594 1971, Chem.Abstr., 77(114701)

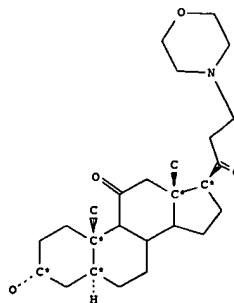
Reaction:

RX
 Reaction ID (.ID): 6377982
 Product BRN (.PBRN): 1182924
 Product (.PRO): 3-hydroxy-21-(2-morpholin-4-yl-ethoxy)-pregnane-11,20-dione
 No. of React. Details (.NVAR): 1

Reaction Details:

L12 ANSWER 9 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 1176237
 Beilstein Pref. RN (BPR): 51228-01-4
 CAS Reg. No. (RN): 51228-01-4
 Chemical Name (CN): 3-hydroxy-23-morpholin-4-yl-21,24-dinor-cholane-11,20-dione
 Autonom Name (AUN): 3-hydroxy-10,13-dimethyl-17-((3-morpholin-4-yl-propionyl)-hexadecahydro-cyclopenta[*a*]phenanthren-11-one
 C26 H41 N O4
 Molec. Formula (MF):
 Molecular Weight (MW): 431.61
 Lawson Number (LN): 30824, 15890
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 1131471
 Tautomer ID (TAUTID): 1150123
 Beilstein Citation (BSO): 5-27
 Entry Date (DED): 1988/11/29
 Update Date (DUPD): 1992/04/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2

L12 ANSWER 9 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Optical Rotatory Power:

Value	Type	Wavelength	Ref.
(ORP)	(.TYP)	(.W)	
(deg)		(nm)	
73	[alpha]	589	1

Reference(s):

1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:

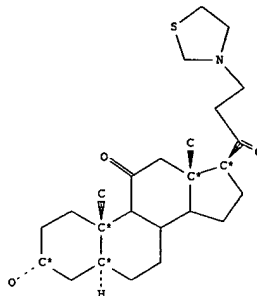
RX
Reaction ID (.ID): 6373933
Product BRN (.PBRN): 1176237
Product (.PRO): 3-hydroxy-23-morpholin-4-yl-21,24-dinor-
cholane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 6373933.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 10 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	1174057
Beilstein Pref. RN (BPR):	51228-28-5
CAS Reg. No. (RN):	51228-28-5
Chemical Name (CN):	3-hydroxy-23-thiazolidin-3-yl-21,24-dinor- cholane-11,20-dione
Autonom Name (AUN):	3-hydroxy-10,13-dimethyl-17-(3-thiazolidin- 3-yl-propionyl)-hexadecahydro- cyclopenta<a>phenanthren-11-one C25 H39 N O3 S
Molec. Formula (MF):	433.65
Molecular Weight (MW):	30831, 15890
Lawson Number (LN):	File Segment (FS):
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1128524
Tautomer ID (TAUTID):	1149485
Beilstein Citation (BSO):	5-27
Entry Date (DED):	1988/11/29
Update Date (DUPD):	1992/04/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1

L12 ANSWER 10 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Optical Rotatory Power:

Value	Type	Wavelength	Ref.
(ORP)	(.TYP)	(.W)	
(deg)		(nm)	
84.5	[alpha]	589	1

Reference(s):

1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

Reaction:

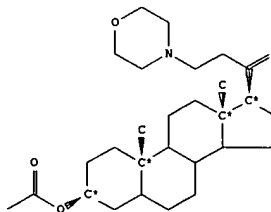
RX
Reaction ID (.ID): 6372577
Product BRN (.PBRN): 1174057
Product (.PRO): 3-hydroxy-23-thiazolidin-3-yl-21,24-dinor-
cholane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 6372577.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab.Ltd. DE 2323950 1973, Chem.Abstr., 80(60089)

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	1047630
Beilstein Pref. RN (BPR):	103572-43-6
CAS Reg. No. (RN):	103572-43-6
Chemical Name (CN):	3-acetoxy-23-morpholin-4-yl-21,24-dinor- cholane-20-one
Autonom Name (AUN):	acetic acid 10,13-dimethyl-17-(3-morpholin- 4-yl-propionyl)-hexadecahydro- cyclopenta<a>phenanthren-3-yl ester C28 H45 N O4
Molec. Formula (MF):	459.67
Molecular Weight (MW):	30824, 15809, 1155
Lawson Number (LN):	File Segment (FS):
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1026819
Tautomer ID (TAUTID):	1046176
Beilstein Citation (BSO):	5-27
Entry Date (DED):	1988/11/29
Update Date (DUPD):	1992/04/07



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

UPD	Update Date	1
CDER	Chemical Derivative	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Chemical Derivative:

CDER
Note(s) (.COM): Hydrochlorid; F: 197-199grad
(Propan-2-ol); <.alpha.>(D): +48.0grad
(Dioxan)

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Melting Point:

Value	Solvent	Ref.
(MP)	(.SOL)	
(Cel)		

92 - 95 |hexane |1

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

Optical Rotatory Power:

Value	Type	Solvent	Wavelen.	Ref.
(ORP)	(.TYP)	(.SOL)	(.W)	
(deg)			(nm)	

56 | |alpha | |dioxane | 589 |1

Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

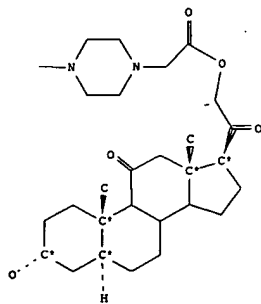
Reaction:

RX
Reaction ID (.ID): 6301110
Product BRN (.PBRN): 1047630
Product (.PRO): 3-acetoxy-23-morpholin-4-yl-21,24-dinor-
cholan-20-one
No. of React. Details (.NVAR): 1

Reaction Details:

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 867726
Beilstein Pref. RN (BPR): 38392-80-2
CAS Reg. No. (RN): 38392-80-2
Chemical Name (CN): 3-hydroxy-21-((4-methyl-piperazin-1-yl)-
acetoxy)-pregnane-11,20-dione,
(4-methyl-piperazin-1-yl)-acetic acid
Autonom Name (AUN): 3-hydroxy-11,20-dioxo-pregnan-21-yl ester
(4-methyl-piperazin-1-yl)-acetic acid
2-(3-hydroxy-10,13-dimethyl-11-oxo-
hexadecahydro-cyclopenta<a>phenanthren-17-
yl)-2-oxo-ethyl ester
Molec. Formula (MF): C28 H44 N2 O5
Molecular Weight (MW): 488.67
Lawson Number (LN): 28000, 9769, 3379, 2817
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 844542
Tautomer ID (TAUTID): 864337
Beilstein Citation (BSO): 5-23
Entry Date (DED): 1988/11/28
Update Date (DUPD): 1989/12/04



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	2
AUN	Autonomname	1

L12 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

RX
Reaction RID (.RID): 6301110.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Merck AG DE 1107662 1959, Chem.Abstr., 56(530), <1962>

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	
(Cel)	

158 - 163 |1

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYP)	(.W)	
(deg)		(nm)	

83 | |alpha | | 589 |1

Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Reaction:

RX
Reaction ID (.ID): 6153907
Product BRN (.PBRN): 867726
Product (.PRO): 3-hydroxy-21-((4-methyl-piperazin-1-yl)-
acetoxy)-pregnane-11,20-dione
No. of React. Details (.NVAR): 1

Reaction Details:

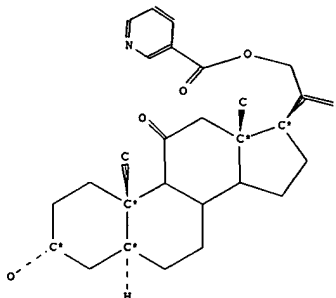
RX
Reaction RID (.RID): 6153907.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):

L12 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 463947
Beilstein Pref. RN (BPR): 38392-72-2
CAS Reg. No. (RN): 38392-72-2
Chemical Name (CN): nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester
Autonom Name (AUN): nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester
Molec. Formula (MF): C27 H35 N O5
Molecular Weight (MW): 453.58
Lawson Number (LN): 26332, 9769
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 454285
Tautomer ID (TAUTID): 472546
Beilstein Citation (BSO): 5-22
Entry Date (DED): 1988/11/28
Update Date (DUPD): 1988/12/08



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Code	Name	Occurrence
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value	Ref.
(MP)	1
(Cel)	1

208 - 211 | 1

Reference(s):

1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Optical Rotatory Power:

Value	Type	Wavelen.	Ref.
(ORP)	(.TYP)	(.W)	1
(deg)	1	(nm)	1

110.5 | [alpha] | 589 | 1

Reference(s):

1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

Reaction:

RX	Reaction ID (.ID):	5666708
	Product BRN (.PBRN):	463947
	Product (.PRO):	nicotinic acid 2-(3-hydroxy-10,13-dimethyl-11-oxo-hexadecahydro-cyclopenta<a>phenanthren-17-yl)-2-oxo-ethyl ester
	No. of React. Details (.NVAR):	1

Reaction Details:

L12 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

RX
Reaction RID (.RID): 5666708.1
Reaction Classification (.CL): Preparation (half reaction)
Reference(s):
1. Patent: Glaxo Lab. DE 2162592 1971, Chem.Abstr., 77(102035)

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FILE 'REGISTRY'. ENTERED AT 11:49:25 ON 23 SEP 2003

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L2 0 S L1
L3 77 S L1 FULL
L4 STRUCTURE UPLOADED
L5 10 S L4 FULL SUB=L3
L6 10 S L4 FULL
L7 STRUCTURE UPLOADED
L8 19 S L7 FULL
L9 29 S L6 OR L8

FILE 'CAPLUS' ENTERED AT 11:59:19 ON 23 SEP 2003

L10 9 S L8

FILE 'BEILSTEIN' ENTERED AT 12:03:14 ON 23 SEP 2003

L11 0 S L4 FULL
L12 13 S L7 FULL

09/321,882

Page 1

=> d ibib ab hitstr 1-7

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS ON STN

ACCESSION NUMBER: 2000:790531 CAPLUS
 DOCUMENT NUMBER: 132:350392
 TITLE: Preparation of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity
 INVENTOR(S): Hogenkamp, Derk L.
 PATENT ASSIGNEE(S): Cocensys, Inc., USA
 SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
VO 2000066614	A1	20001109	VO 2000-US11680	20000428
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000010060	A	20020115	BR 2000-10060	20000428
EP 1177206	A1	20020206	EP 2000-930250	20000428
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002543218	T2	20021217	JP 2000-615643	20000428
NO 2001005262	A	20011219	NO 2001-5262	20011026
PRIORITY APPLN. INFO.: US 1999-131578P P 19990429 WO 2000-US11680 W 20000428				

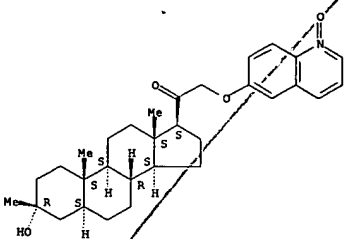
AB 3.alpha.-Hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids I (R1 = H, Me; R2 = 5.alpha.- or 5.beta.-H; R3 = optionally substituted N-attached heteroaryl group or -XR4 where R4 = optionally substituted carbon-attached heteroaryl group; X = O, S, N) or a pharmaceutically acceptable salt, prodrug or solvate thereof were prepd. Thus II was prepd. from 3.alpha.-hydroxy-3.beta.-methoxymethyl-5.alpha.-pregnan-20-one and imidazole which was then converted to the hydrochloride salt. Steroids I are useful as anticonvulsants, sedative/hypnotics and anesthetics [no data].

IT 304910-83-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity)

RN 304910-83-6 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-(6-quinolinyl)oxy-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

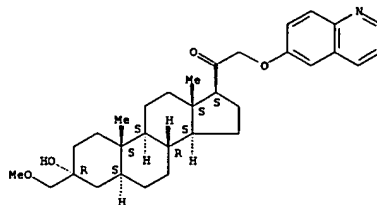
Absolute stereochemistry.

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

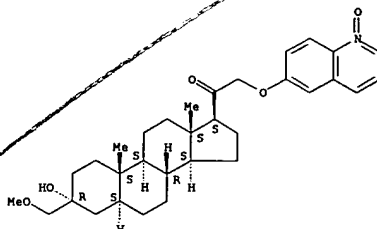
L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)



IT 256955-85-8P 304910-84-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 3.alpha.-hydroxy-3.beta.-methoxymethyl-21-heterocyclic substituted steroids with anesthetic activity)

RN 256955-85-8 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 304910-84-7 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS ON STN

ACCESSION NUMBER: 1999:778442 CAPLUS
 DOCUMENT NUMBER: 132:132237
 TITLE: Response-rate suppression in operant paradigm as predictor of soporific potency in rats and identification of three novel sedative-hypnotic neuroactive steroids
 AUTHOR(S): Vanover, Kimberly E.; Edgar, Dale M.; Seidel, Wesley F.; Hogenkamp, Derk J.; Fick, David B.; Lan, Nancy C.; Gee, Kelvin W.; Carter, Richard B.
 CORPORATE SOURCE: Cocensys, Inc., Irvine, CA, USA
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (1999), 291(3), 1317-1323
 CODEN: JPETAB; ISSN: 0022-3565
 PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
 DOCUMENT TYPE: Journal
 LANGUAGE: English

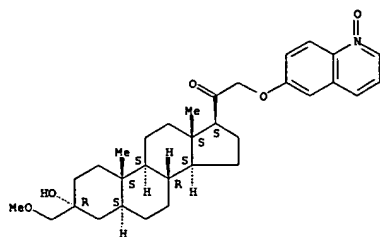
AB Novel neuroactive steroids were evaluated for their effects on operant responding, rotarod motor performance, and EEG recording in rats. Co 134444, Co 177843, and Co 127501 were compared with the prototypical .gamma.-aminobutyric acidA-pos. allosteric modulators triazolam, zolpidem, pentobarbital, pregnanolone, and CCD 3693. Each of the compds. produced a dose-related decrease in response rates under a variable-interval 2-min schedule of pos. reinforcement in an operant paradigm. In addn., all compds. produced a dose-related increase in ataxia and significant increases in nonrapid eye movement sleep in this expt. or have been previously reported to do so. Co 134444, Co 177843, and Co 127501 increased nonrapid eye movement sleep at doses that had no effect on rapid eye movement sleep. All of the compds. were more potent at decreasing operant responding than they were at increasing ataxia. Furthermore, the potency of compds. to produce response-rate suppression in an operant paradigm appeared to be a better predictor of soporific potency than did potency in the rotarod assay. The screening for sedative-hypnotic activity resulted in the identification of the novel orally active neuroactive steroids Co 134444, Co 177843, and Co 127501.

IT 256955-85-8, Co 177843
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (response-rate suppression in operant paradigm as predictor of soporific potency: novel sedative-hypnotic neuroactive steroids identification)

RN 256955-85-8 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-(methoxymethyl)-21-[(1-oxido-6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:450892 CAPLUS
 DOCUMENT NUMBER: 131:102428
 TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
 INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
 PATENT ASSIGNEE(S): Cocensys, Inc., USA
 SOURCE: U.S., 28 pp.
 CODEN: USXKAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5925630	A	19990720	US 1996-659192	19960606
CA 2223996	AA	19961219	CA 1996-2223996	19960606
CN 1190404	A	19980812	CN 1996-195360	19960606
EP 1288220	A2	20030305	EP 2002-25321	19960606

R: AL, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, SI, LT, LV, FI, AE

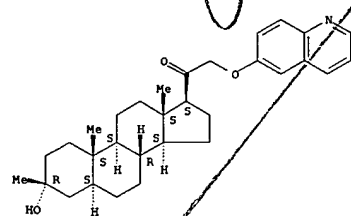
PRIORITY APPL. INFO.: US 1995-467404 A2 19950606
 EP 1996-919372 A3 19961219

OTHER SOURCE(S): MARPAT 131:102428
 AB Neuroactive steroids of formula I (R = H, NH2, thio, sulfinyl, sulfonyl, halo, alkoxy, alkyl, alkenyl, alkynyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, chaloalkyl, aryl, etc.; R2 = H, alkoxy, keto, Me; R3 = alkoxy, alkenyloxy, alkynyloxy; R4 = H, Me; R5 = H, absent; R6 = H, alkanoyl, etc.; R7 = H, halo, OH, alkoxy, etc.; R8 = H, halo; R9 = H, halo, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halo, alkyl, OH, alkoxy, CN, etc.) are prep'd. These derivs. are capable of acting at a recently identified site on the GABA receptor complex (GRC), thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.β-methoxy-5.β-androstan-3-one to give II. II protected 87.5% of mice injected with metrazol from convulsions.

IT 186264-63-1P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of neuroactive steroids of androstane and pregnane series)
 RN 186264-63-1 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.α.,5.α.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:112239 CAPLUS
 DOCUMENT NUMBER: 128:188632
 TITLE: Use of GABA agonists and NMDA receptor antagonists for the treatment of migraine headache
 INVENTOR(S): Lan, Nancy C.
 PATENT ASSIGNEE(S): Cocensys, Inc., USA; Lan, Nancy C.
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9805337	A1	19980212	WO 1997-US13430	19970731

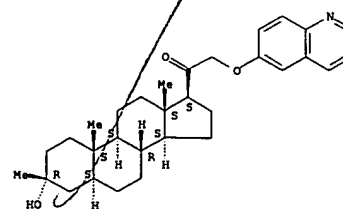
V: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GR, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LR, LU, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, ST, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, BG, BR, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9739672 A1 19980225 AU 1997-39672 19970731
 US 1996-229372 P 19960801
 WO 1997-US13430 W 19970731

AB Methods are disclosed for treating or preventing migraine headache by administering to an animal a GABA receptor agonist (e.g. a neuroactive steroid) and/or an NMDA receptor antagonist (e.g. a dihydroquinoline deriv.). Also disclosed are pharmaceutical compns. and kits for the treatment or prevention of migraine headache.

IT 186264-63-1 203719-40-8
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (GABA agonists and NMDA receptor antagonists for migraine headache treatment)
 RN 186264-63-1 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.α.,5.α.)-(9CI) (CA INDEX NAME)

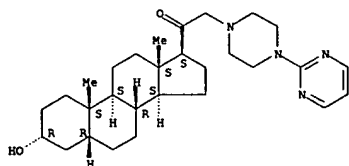
Absolute stereochemistry.



L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 203719-40-8 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-21-[(4-(2-pyrimidinyl)-1-piperazinyl)-, (3.alpha.,5.beta.)-] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:113460 CAPLUS
 DOCUMENT NUMBER: 126:131695
 TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
 INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
 PATENT ASSIGNEE(S): Cocensys, Inc., USA
 SOURCE: PCT Int. Appl., 94 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640043	A2	19961219	WO 1996-US10115	19960606
WO 9640043	A3	19970327		
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
CA 2223996	AA	19961219	CA 1996-2223996	19960606
AU 9661725	A1	19961230	AU 1996-61725	19960606
AU 725214	B2	20001005		
EP 837874	A2	19980429	EP 1996-919372	19960606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1190404	A	19980812	CN 1996-195360	19960606
BR 9608592	A	19990629	BR 1996-8592	19960606
JP 11507643	T2	19990706	JP 1997-502210	19960606
RU 2194712	C2	20021220	RU 1998-100755	19960606
EP 1288220	A2	20030305	EP 2002-25321	19960606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL				
NO 9705608	A	19980206	NO 1997-5608	19971204
FI 9704448	A	19971205	FI 1997-4448	19971205
PRIORITY APPLN. INFO.: US 1995-467404 A 19950606				
WO 1996-US10115 W 19960606				
EP 1996-919372 A3 19961219				

OTHER SOURCE(S): MARPAT 126:131695
 AB Comps. of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halogen, alkoxy, alkyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R2 = H, OH, alkoxy, alkanoyloxy, carbalkoxy, keto, amino; R3 = H, alkoxy, alkenyloxy, etc.; R4 = H, alkyl; R5 = H, absent; R6 = H, alkanoyl, aminocarbonyl, alkoxy, carbonyl; R7 = H, halogen, OH, alkoxy, alkanoyloxy, carbalkoxy; R8 = H, halogen; R9 = H, halogen, alkyl, alkoxy, arylalkoxy, amino; R10 = H, halogen, OH, alkyl, etc.] are prepd. as neuroactive prodrugs, due to their ability to modulate the GABAA receptor-chloride ionophore complex. These derivs. are capable of acting at a recently identified site on the GRC, thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.beta.-methoxy-

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

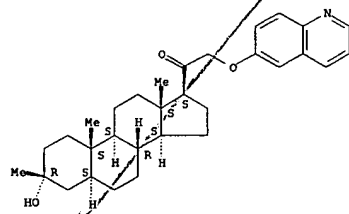
5.beta.-androstane-3-one to give II. II (10 mg/kg IP) protected 87.5% of mice injected with metrazol from convulsions.

IT 186264-63-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of neuroactive androstanes and pregnanes)

RN 186264-63-1 CAPLUS
 CN Pregnan-20-one, 3-hydroxy-3-methyl-21-[(6-quinolinyl)oxy]-, (3.alpha.,5.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1988:631361 CAPLUS
 DOCUMENT NUMBER: 109:231361
 TITLE: Amino steroids useful for treating a variety of conditions, and a process for their preparation
 INVENTOR(S): McCall, John M.; Ayer, Donald E.; Jacobsen, E. Jon; Van Doorick, Frederick J.; Palmer, John R.; Karnes, Harold A.
 PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: Eur. Pat. Appl., 90 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 263213	A1	19880413	EP 1986-307808	19861009
EP 263213	B1	19950906		
R: AT, ES, GR				
ES 2078890	T3	19960101	ES 1986-307808	19861009
PRIORITY APPLN. INFO.: EP 1986-307808 19861009				
OTHER SOURCE(S): CASREACT 109:231361; MARPAT 109:231361				

AB Various amino-substituted steroids were prepd. for use in the treatment of a wide variety of conditions. Aminolysis of 21-iodo-16.alpha.-methylpregna-1,4,9(11)-triene-3,20-dione by 1-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)piperazine in MeCN contg. K2CO3 at 60.degree., followed by chromatog. and salification with MeSO3H, gave the amino steroid dimethanesulfonate I. In the in vivo mouse head injury test of Hall, 3 mg I/kg increases 1-h post-injury grip test scores by 134.5%.

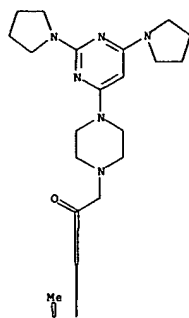
IT 111641-00-OP 111641-01-1P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as drug)

RN 111641-00-0 CAPLUS
 CN Pregnan-20-one, 21-[(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.beta.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

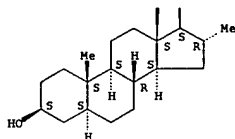
Absolute stereochemistry.

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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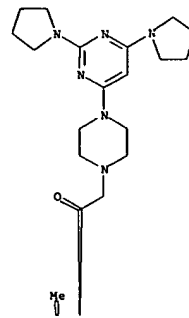


RN 111641-01-1 CAPLUS
 CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.alpha.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

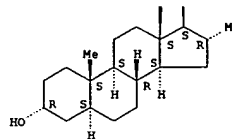
Absolute stereochemistry.

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN

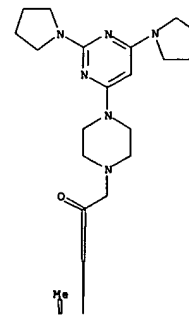
ACCESSION NUMBER: 1988:6287 CAPLUS
 DOCUMENT NUMBER: 108:6287
 TITLE: Amino-substituted steroids having a variety of pharmacological activities, and processes for their preparation
 INVENTOR(S): McCall, John M.; Jacobsen, E. Jon; Van Doornik, Frederick J.; Palmer, John R.; Karnes, Harold A.
 PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: PCT Int. Appl., 169 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8701706	A2	19870326	WO 1986-US1797	19860828
WO 8701706	A3	19870716		
W: AU, DK, FI, JP, KR, NO, SU, US, US, US, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
IL 79702	A1	19920216	IL 1986-79702	19860812
IL 98007	A1	19920216	IL 1986-98007	19860812
ZA 8606097	A	19880330	ZA 1986-6097	19860813
CA 1308707	A1	19921013	CA 1986-516177	19860818
AU 8663356	A1	19870407	AU 1986-63356	19860828
AU 593284	B2	19900208		
EP 238545	A1	19870930	EP 1986-905605	19860828
EP 238545	B1	19951115		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 63500868	T2	19880331	JP 1986-504810	19860828
JP 05035158	B4	19930525		
AT 130307	E	19951215	AT 1986-905605	19860828
CN 86106226	A	19870318	CN 1986-106226	19860912
CN 1030319	B	19951122		
DK 8702375	A	19870511	DK 1987-2375	19870511
NO 8701930	A	19870511	NO 1987-1930	19870511
NO 176762	B	19950213		
NO 176762	C	19950531		
FI 8702107	A	19870512	FI 1987-2107	19870512
FI 94417	B	19950531		
FI 94417	C	19950531		
US 5099019	A	19920324	US 1988-229675	19880808
AU 8940806	A1	19891207	AU 1989-40806	19890825
AU 614661	B2	19910905		
AU 8940807	A1	19891207	AU 1989-40807	19890825
AU 614418	B2	19910829		
US 5175281	A	19921229	US 1991-749830	19910826
US 5322943	A	19940621	US 1991-749829	19910826
JP 05112597	A2	19930507	JP 1992-8426	19920121
US 35053	E	19951010	US 1992-959310	19921009
US 5268477	A	19931207	US 1992-977768	19921119
US 5380839	A	19950110	US 1992-983082	19921201
US 5380840	A	19950110	US 1992-983084	19921201
US 5380841	A	19950110	US 1992-984299	19921201
US 5382661	A	19950117	US 1992-984298	19921201
US 5506354	A	19960409	US 1992-984302	19921201
PRIORITY APPLN. INFO.:			US 1985-775204	19850912
			US 1985-811058	19851219
			US 1986-877287	19860623

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

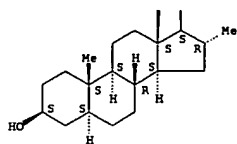
US 1986-888231 19860729
 IL 1986-79702 19860812
 WO 1986-US1797 19860828
 US 1987-121822 19870511
 US 1988-227812 19880803
 US 1988-229675 19880808
 US 1991-749829 19910826
 US 1991-749830 19910826
 AB Numerous pregnane derivs. with amino-substituted sidechains were prepd. for use as various types of drugs. Aminolysis of 21-iodo-16.alpha.-methylpregna-1,4,9(11)-triene-3,20-dione with 4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)piperazine in MeCN contg. K2CO3 at 60.degree. gave [[bis(pyrrolidino)pyrimidinyl]piperazinyl]pregnane deriv. I, which was converted to I.2MeSO3H (II). In the interleukin-1-induced T-cell proliferation assay, II gave 62% inhibition at 10-6 M, thereby demonstrating antiarthritic activity.
 IT 111641-00-0P 111641-01-1P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as drug)
 RN 111641-00-0 CAPLUS
 CN Pregnan-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-3-hydroxy-16-methyl-, (3.beta.,5.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)
 Absolute stereochemistry.

PAGE 1-A



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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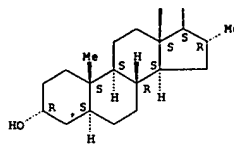


RN 111641-01-1 CAPLUS
 CN Pregnen-20-one, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-
 3-hydroxy-16-methyl-, (3.alpha.,5.alpha.,16.alpha.)- (9CI) (CA INDEX
 NAME)

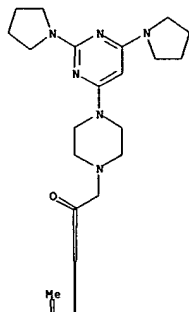
Absolute stereochemistry.

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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FILE 'REGISTRY' ENTERED AT 14:17:37 ON 23 SEP 2003

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 138 S L1 FULL

L4 7 S L3 AND (PYRIDY? OR PYRIMIDINY? OR PYRAZINY? OR IMIDAZOLY? OR

FILE 'CAPLUS' ENTERED AT 14:20:52 ON 23 SEP 2003

L5 7 S L4

FILE 'BEILSTEIN' ENTERED AT 14:22:13 ON 23 SEP 2003

L6 0 S L4 FULL

L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:113460 CAPLUS
 DOCUMENT NUMBER: 126:131695
 TITLE: Preparation of neuroactive steroids of the androstane and pregnane series
 INVENTOR(S): Upasani, Ravindra B.; Fick, David B.; Hogenkamp, Derk J.; Lan, Nancy C.
 PATENT ASSIGNEE(S): Cocensys, Inc., USA
 SOURCE: PCT Int. Appl., 94 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

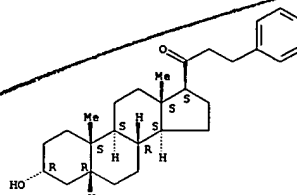
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9640043	A2	19961219	WO 1996-US10115	19960606
WO 9640043	A3	19970327		
V: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LA, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CG, CI, CM, GA, GN				
CA 2223996	AA	19961219	CA 1996-2223996	19960606
AU 9661725	A1	19961230	AU 1996-61725	19960606
AU 725214	B2	20001005		
EP 837874	A2	19980429	EP 1996-919372	19960606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1190404	A	19980812	CN 1996-195160	19960606
BR 9608592	A	19990629	BR 1996-8592	19960606
JP 11507643	T2	19990706	JP 1997-502210	19960606
RU 2194712	C2	20021220	RU 1998-100755	19960606
EP 1288220	A2	20030305	EP 2002-25321	19960606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, AL				
NO 9705608	A	19980206	NO 1997-5608	19971204
FI 9704448	A	19971205	FI 1997-4448	19971205
PRIORITY APPL. INFO.: US 1995-467404 A 19950606 WO 1996-US10115 W 19960606 EP 1996-919372 A3 19961219				

OTHER SOURCE(S): MARPAT 126:131695
 AB Comps. of formula I [R = H, NH2, thio, sulfinyl, sulfonyl, halogen, alkoxy, alkyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, aryl, etc.; R2 = H, OH, alkoxy, alkenyloxy, carbalkoxy, keto, amino; R3 = H, alkoxy, alkenyloxy, etc.; R4 = H, alkyl; R5 = H, absent; R6 = H, alkanoyl, aminocarbonyl, alkoxy, carbonyl; R7 = H, halogen, OH, alkoxy, alkanoyloxy, carbalkoxy; R8 = H, halogen; R9 = H, halogen, alkyl, alkoxy, acylalkoxy, amino; R10 = H, halogen, OH, alkyl, etc.] are prep. as neuroactive produgs, due to their ability to modulate the GABA_A receptor-chloride ionophore complex. These derivs. are capable of acting at a recently identified site on the GRC, thereby modulating brain excitability in a manner that will alleviate stress, anxiety, insomnia, mood disorders that are amenable to GRC-active agents (such as depression) and seizure activity. Thus, 2-methyl-1-buten-3-yne was added to 17.β-methoxy-

L10 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

5.β-androstan-3-one to give II. II (10 mg/kg IP) protected 87.5% of mice injected with metrazol from convulsions.
 IT 186264-69-79
 AL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of neuroactive androstanes and pregnanes)
 RN 186264-69-7 CAPLUS
 CN 1-Propanone, 1-[(3.α.,5.β.,17.β.)-3-hydroxyandrostan-17-yl]-3-(4-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



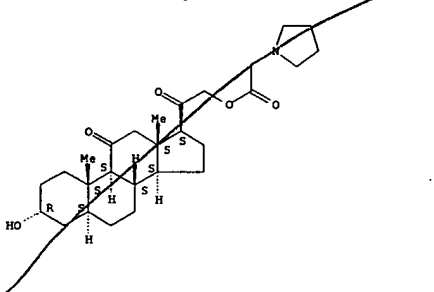
L10 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1975:558163 CAPLUS
 DOCUMENT NUMBER: 83:158163
 TITLE: Structure-activity relations in steroidal anesthetics
 AUTHOR(S): Philipps, G. H.
 CORPORATE SOURCE: Org. Chem. Dep., Glaxo Res. Ltd., Greenford/Middlesex, UK
 SOURCE: Journal of Steroid Biochemistry (1975), 6(5), 607-13
 CODEN: JSTBBK; ISSN: 0022-4731
 DOCUMENT TYPE: Patent
 LANGUAGE: English

AB The introduction of double bonds and substituents into Alphaxalone [23930-19-0] modify its anesthetic activity, as detd. in mice, and these modifications are discussed with particular ref. to the conformation of the A-ring. A variety of side chains may be present at the 17.β-position. Some water-sol. steroids which show instantaneous induction of anesthesia are described.

IT 56857-38-6
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (anesthetic activity of)
 RN 56857-38-6 CAPLUS
 CN Pregnane-11,20-dione, 3-hydroxy-21-[(1-pyrrolidinylacetyl)oxy]-, (3.α.,5.α.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1974:60089 CAPLUS
 DOCUMENT NUMBER: 80:60089
 TITLE: 3.α.-Hydroxy-5.α.-pregnanes
 INVENTOR(S): Phillips, Gordon Hanley; Lawrence, Robin; Stephenson, Leslie; Ayres, Barry E.
 PATENT ASSIGNEE(S): Glaxo Laboratories Ltd.
 SOURCE: Ger. Offen., 75 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

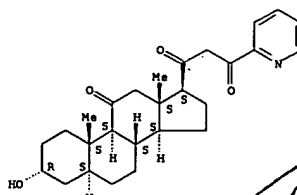
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2323950	A1	19731213	DE 1973-2323950	19730511
US 3998829	A	19761221	US 1973-358381	19730508
BE 799433	A1	19731112	BE 1973-131031	19730511
NL 7306606	A	19731114	NL 1973-6606	19730511
FR 2184711	A1	19731228	FR 1973-17079	19730511
JP 49048652	A2	19740511	JP 1973-52424	19730511
ZA 7303218	A	19740529	ZA 1973-3218	19730511
AU 7355616	A1	19741114	AU 1973-55616	19730511
GB 1436324	A	19760519	GB 1972-22489	19730511
DK 135775	B	19770620	DK 1973-2604	19730511
CA 1014947	A1	19770802	CA 1973-171026	19730511

PRIORITY APPL. INFO.: GB 1972-22489 19720512
 AB Hydroxypregnanes I, II (R = H, alkyl, acyl; R1 = H; R2 = CH2, CH2CH2, or R2 = H, R3 = alkoxy, alkylthio, acyl, acyloxy, acylthio, morpholino, halo, Me; R2 = R3 = Me) (45 compds.) were prep. from I and II (R = R1 = H; R2R3 = CH2; R2 = H, R3 = CH2OH) by Claisen condensation with active methylene compds. Thus, 1 g I (R = R1 = H) was treated with AcOEt-NaH to give 0.5 g I (R1 = Ac).

IT 51227-92-0P 51228-01-4P 51228-28-5P
 51228-32-1P 51228-33-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 51227-92-0 CAPLUS
 CN 1,3-Propanedione, 1-[(3.α.,5.α.,17.β.)-3-hydroxy-11-oxoandrostan-17-yl]-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 51228-01-4 CAPLUS